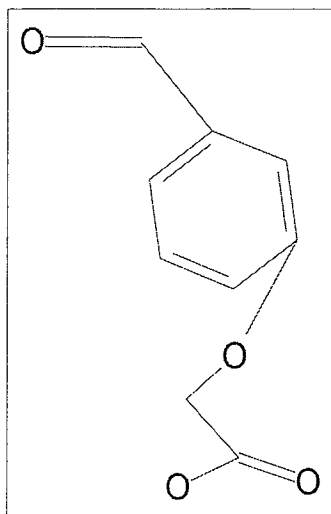


# EXHIBIT A



## Substance Identification

Beilstein Registry Number	<b>2048742</b>
Beilstein Preferred RN	37748-09-7
CAS Registry Number	37748-09-7
Chemical Name	(3-formyl-phenoxy)-acetic acid
Autoname	(3-formyl-phenoxy)-acetic acid
Molecular Formula	C <sub>9</sub> H <sub>8</sub> O <sub>4</sub>
Molecular Weight	180.16
Lawson Number	8629, 1771
Type of Substance	isocyclic
Constitution ID	1856203
Tautomer ID	1952560
Beilstein Reference	0-08-00-00060, 2-08-00-00054, 5-08, 6-08

## Field Availability List 1-6

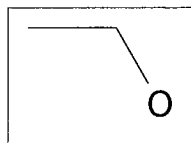
Code	Field Name	Occ.
<u><b>RX</b></u>	Reaction	17
<u><b>CDER</b></u>	Derivative	4
<u><b>CPD</b></u>	Crystal Property Description	1
<u><b>MP</b></u>	Melting Point	5
<u><b>IR</b></u>	IR Spectroscopy	1
<u><b>CNR</b></u>	Reference	16

## Reaction 1 of 17

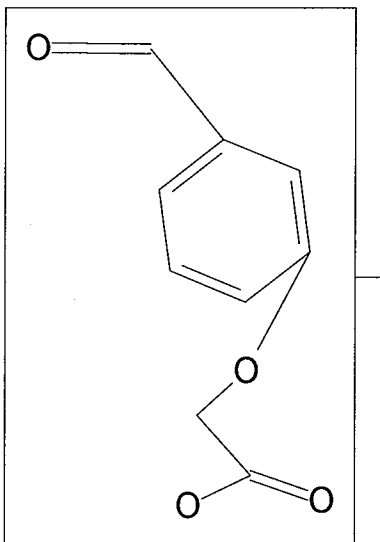
Reaction ID	<u><b>190141</b></u>
Reactant BRN	<u><b>1718733</b></u> ethanol <b>2048742</b> (3-formyl-phenoxy)-acetic acid
Product BRN	<u><b>2109732</b></u> (3-formyl-phenoxy)-acetic acid ethyl ester
No. of Reaction Details	1
Reaction Classification	Preparation
Reagent	HCl
Find similar reactions	<u><b>click here</b></u>

Note 1  
Ref. 1

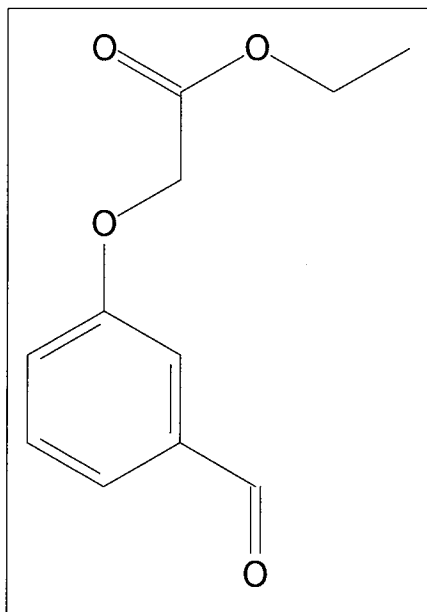
Handbook  
**1970630**; Journal; Elkan; CHBEAM; Chem. Ber.; 19; 1886; 3051.



Reactant 1



Reactant 2



Product 1

## Reaction 2 of 17

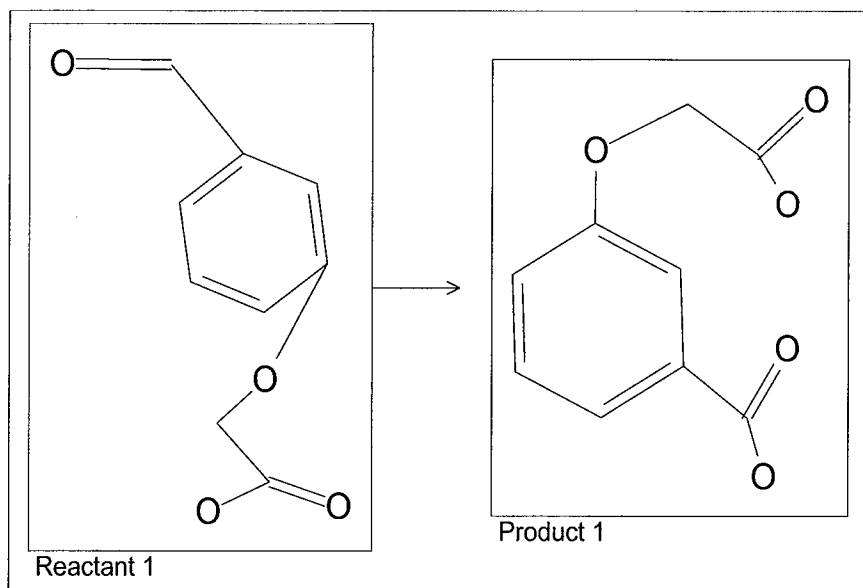
Reaction ID  
Reactant BRN  
Product BRN  
No. of Reaction Details  
Reaction Classification  
Reagent

**309586**  
**2048742** (3-formyl-phenoxy)-acetic acid  
**2695071** 3-carboxymethoxy-benzoic acid  
1  
Preparation  
alkali  
water  
permanganate  
[\*\*click here\*\*](#)

Find similar reactions

Note 1  
Ref. 1

Handbook  
**1970630**; Journal; Elkan; CHBEAM; Chem. Ber.; 19; 1886; 3051.



### Reaction 3 of 17

Reaction ID

Reactant BRN

Product BRN

No. of Reaction Details

Reaction Classification

Reagent

Find similar reactions

**558896**

**2048742** (3-formyl-phenoxy)-acetic acid

**385737** acetic acid anhydride

**3305754** 3-carboxymethoxy-cinnamic acid

1

Preparation

sodium acetate

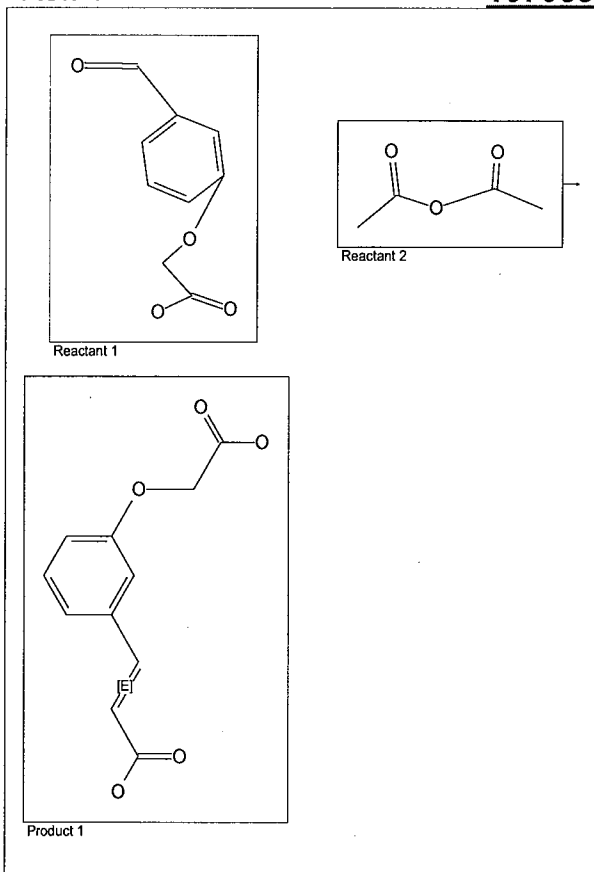
[\*\*click here\*\*](#)

Note 1

Ref. 1

Handbook

**1970630**; Journal; Elkan; CHBEAM; Chem. Ber.; 19; 1886; 3051.



## Reaction 4 of 17

Reaction ID

Reactant BRN

Product BRN

No. of Reaction Details

Reaction Classification

Reagent

Find similar reactions

**636552**

**2048742** (3-formyl-phenoxy)-acetic acid

**505984** acetaldehyde

**3279177** [3-(3-oxo-propenyl)-phenoxy]-acetic acid

1

Preparation

diluted NaOH-solution

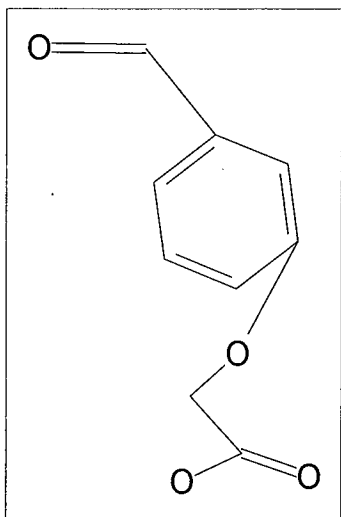
[\*\*click here\*\*](#)

Note 1

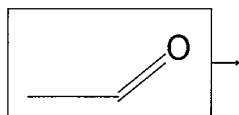
Ref. 1

Handbook

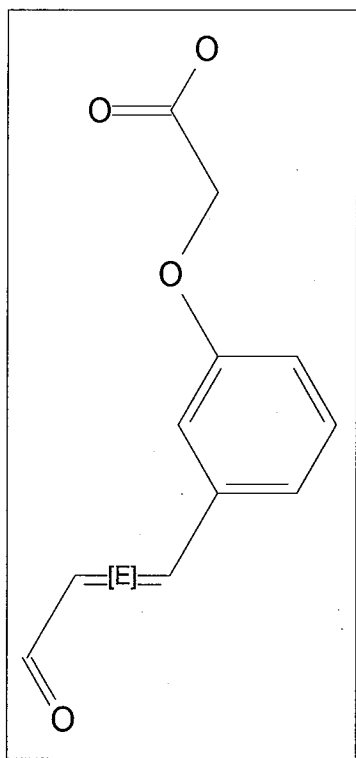
**1970630**; Journal; Elkan; CHBEAM; Chem. Ber.; 19; 1886; 3051.



Reactant 1



Reactant 2



Product 1

## Reaction 5 of 17

Reaction ID  
Reactant BRN

Product BRN  
No. of Reaction Details  
Reaction Classification  
Find similar reactions

**660365**

**605438** chloroacetic acid

**5789338** Pyridinsalz des Oxymaleinsaeureanhydrids

**507099** 3-hydroxy-benzaldehyde

**2048742** (3-formyl-phenoxy)-acetic acid

1

Chemical behaviour

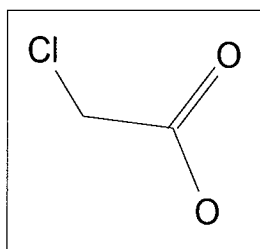
[\*\*click here\*\*](#)

Note 1

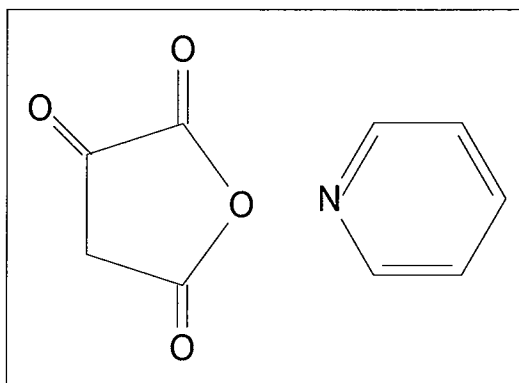
Ref. 1

Handbook

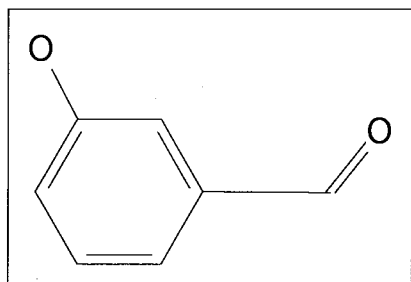
**1970630**; Journal; Elkan; CHBEAM; Chem. Ber.; 19; 1886; 3051.



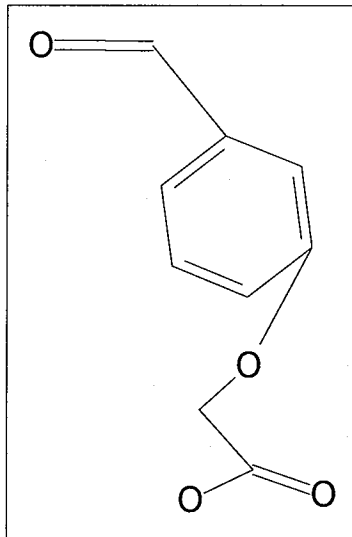
Reactant 1



Reactant 2



Reactant 3



Product 1

## Reaction 6 of 17

Reaction ID  
Reactant BRN

Product BRN  
No. of Reaction Details  
Reaction Classification  
Reagent

**660366**

**507099** 3-hydroxy-benzaldehyde

**605438** chloroacetic acid

**2048742** (3-formyl-phenoxy)-acetic acid

1

Preparation

NaOH-solution

Find similar reactions

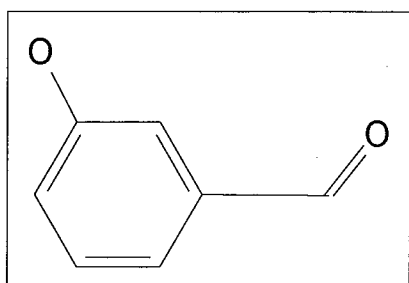
[click here](#)

Note 1

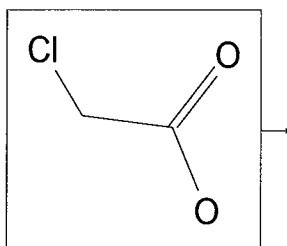
Ref. 1

Handbook

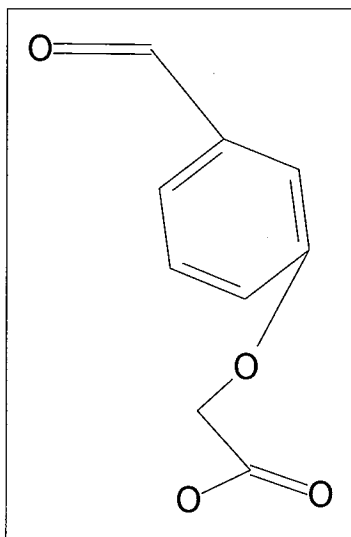
**1970630**; Journal; Elkan; CHBEAM; Chem. Ber.; 19; 1886; 3051.



Reactant 1



Reactant 2



Product 1

## **Reaction 7 of 17**

Reaction ID

Reactant BRN

Product BRN

No. of Reaction Details

Reaction Classification

Reagent

Find similar reactions

**2071867**

**5362023** C<sub>104</sub>H<sub>148</sub>F<sub>12</sub>O<sub>20</sub>

**2048742** (3-formyl-phenoxy)-acetic acid

**6173350** C<sub>140</sub>H<sub>172</sub>F<sub>12</sub>O<sub>32</sub>

1

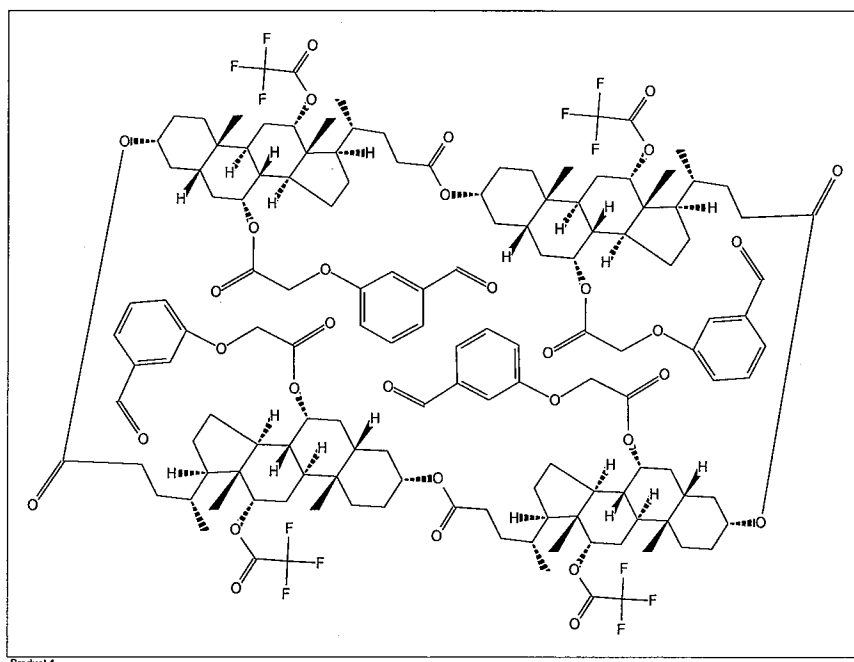
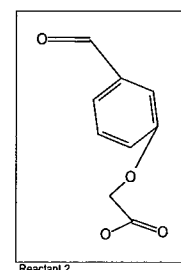
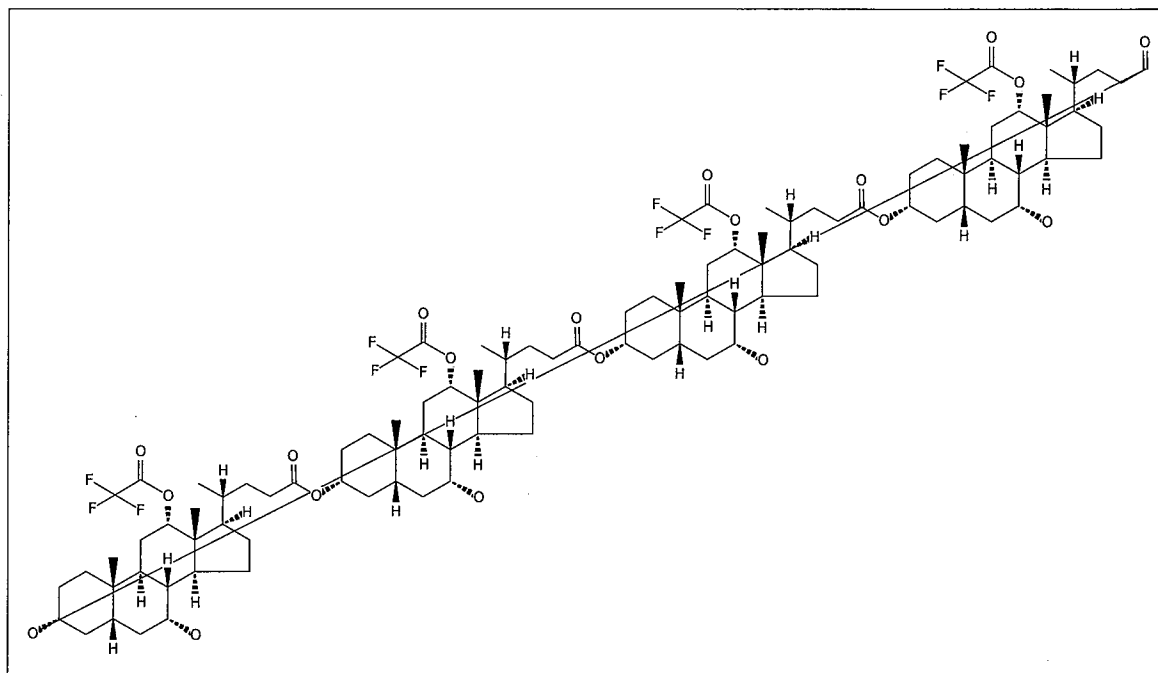
Preparation

dicyclohexylcarbodiimide, DMAP

not available

Ref. 1

**5752565**; Journal; Bonar-Law, Richard P.; Mackay, Lindsey G.; Sanders, Jeremy K. M.; JCCCAT; J. Chem. Soc. Chem. Commun.; EN; 5; 1993; 456-458.



## Reaction 8 of 17

Reaction ID  
Reactant BRN

Product BRN  
No. of Reaction Details  
Reaction Classification  
Other Conditions  
Find similar reactions

**4228398**

**2048742** (3-formyl-phenoxy)-acetic acid

**506236** 1-nitro-propane

**1994538** [3-(2-nitro-but-1-enyl)-phenoxy]-acetic acid

1

Preparation

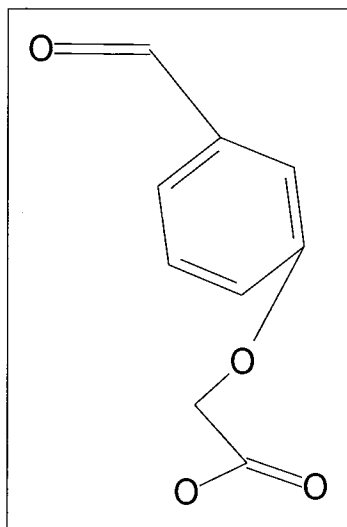
(i) nBuNH<sub>2</sub>, benzene, (ii) /BRN= 506236/, AcOH

[click here](#)

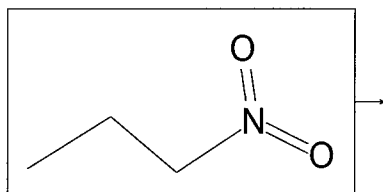
Note 1

Multistep reaction

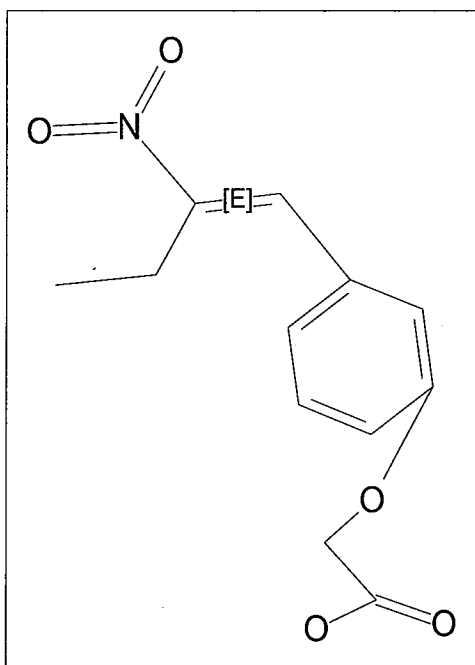




Reactant 1



Reactant 2



Product 1

## Reaction 9 of 17

Reaction ID

Reactant BRN

Product BRN

No. of Reaction Details

Reaction Classification

Reagent

Time

Find similar reactions

**4510213****2048742** (3-formyl-phenoxy)-acetic acid**1159** pyrrole**7564396** {3-[10,15,20-tris-(3-carboxymethoxy-phenyl)-porphyrinogen-5-yl]-phenoxy}-acetic acid

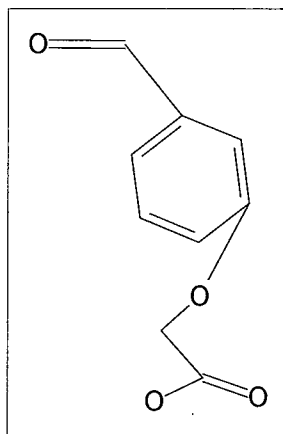
1

Preparation

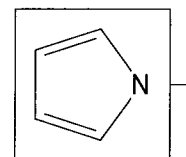
aq. sodium dodecyl sulfate, HCl

2 hour(s)

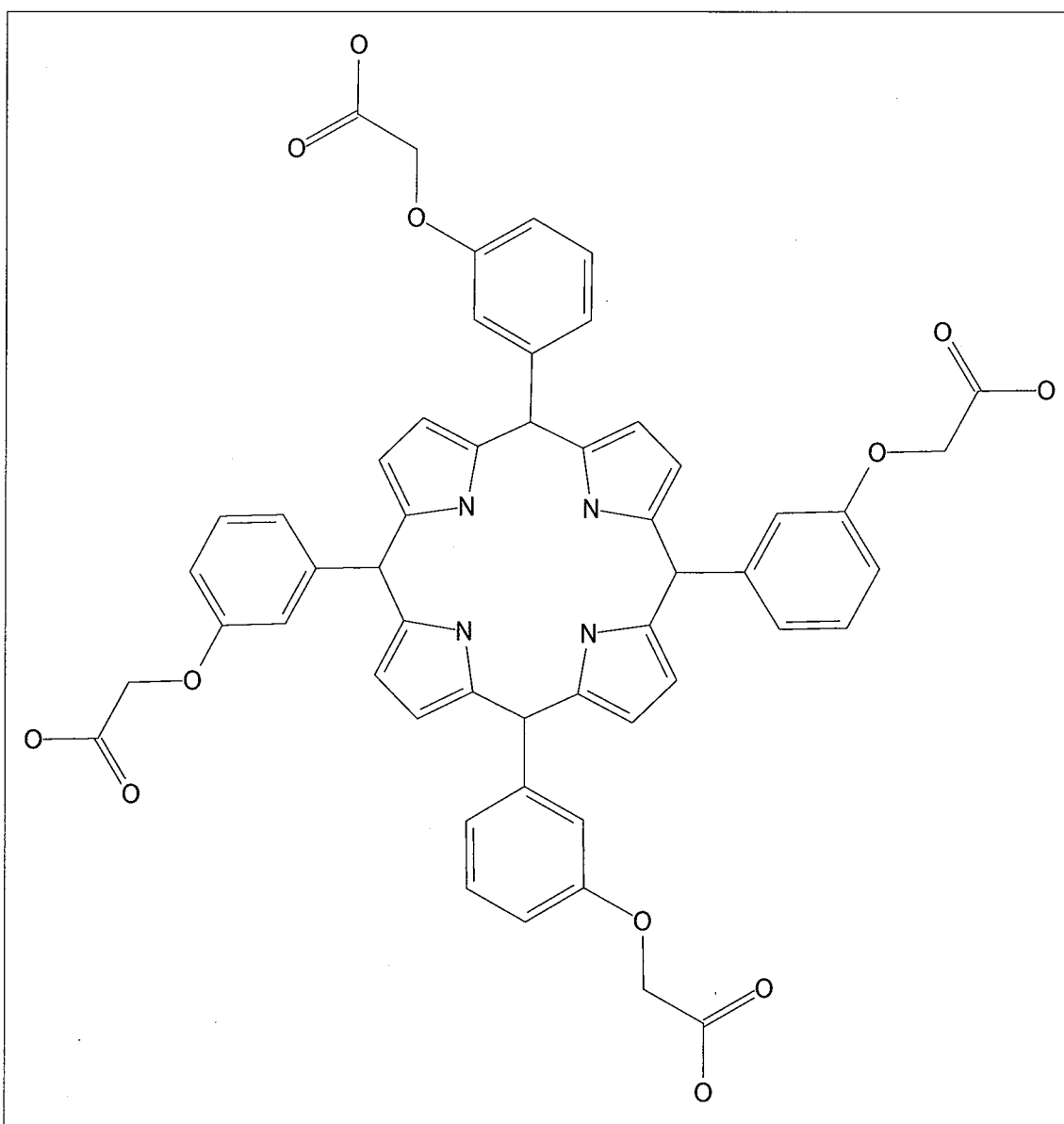
**[click here](#)**



Reactant 1



Reactant 2



Product 1

## Reaction 10 of 17

Reaction ID

Reactant BRN

Product BRN

No. of Reaction Details

Reaction Classification

Reagent

Solvent

**4517320**

**1960557** Methyl-m-formyl-phenoxyacetat

**2048742** (3-formyl-phenoxy)-acetic acid

1

Preparation

aq. KOH

methanol

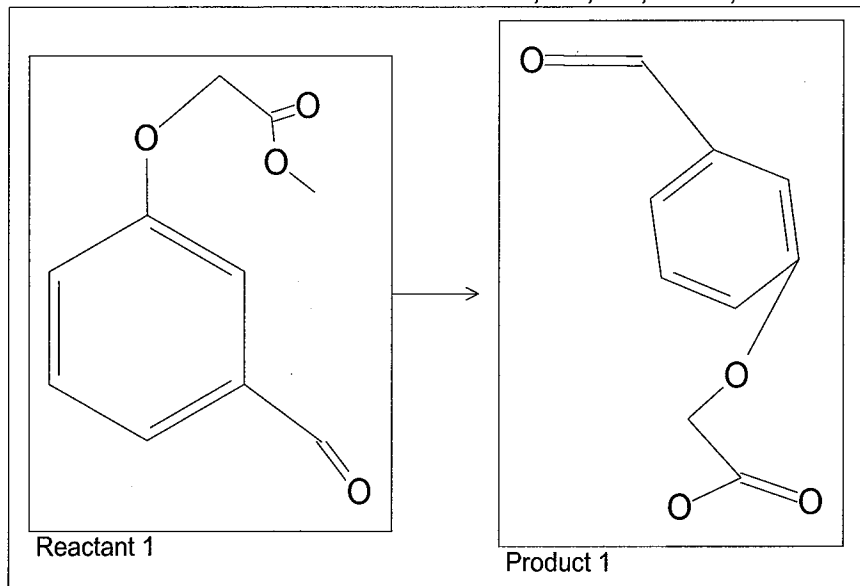
tetrahydrofuran

Find similar reactions

[\*\*click here\*\*](#)

Ref. 1

**6021620**; Journal; Bonar-Law, Richard P.; JOCEAH; J. Org. Chem.; EN; 61; 11; 1996; 3623-3634.



## Reaction 11 of 17

Reaction ID

Reactant BRN

No. of Reaction Details

Reaction Classification

Other Conditions

Find similar reactions

**7149987**

**969616** phenol

**2048742** (3-formyl-phenoxy)-acetic acid

1

Chemical behaviour (half reaction)

durch Kondensation

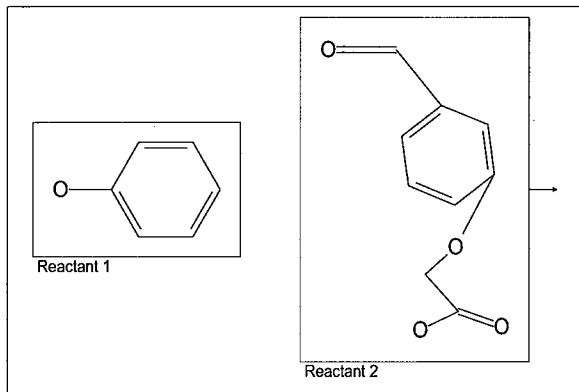
not available

Note 1

Ref. 1

Handbook

**1979953**; Patent; Hoechst Farb.; DE 362382; FTFVA6; Fortschr. Teerfarbenfabr. Verw. Industriezweige; DE; GE; 14; 1160.



## Reaction 12 of 17

Reaction ID

Product BRN

No. of Reaction Details

Reaction Classification

Find similar reactions

7252880

2048742 (3-formyl-phenoxy)-acetic acid

1

Preparation (half reaction)

not available

Ref. 1

4068762; Patent; Biorex Lab. Ltd.; DE 2810253; 1978; Chem.Abstr.; EN; 90; 22628.

Ref. 2

4084581; Patent; Ciba-Geigy; DE 2209128; 1972; Chem.Abstr.; EN; 78; 5413.

Ref. 3

4162241; Journal; Krassowska et al.; PRCHAB; Przem. Chem.; 52; 1973; 741,742,743.

Ref. 4

2893918; Patent; Upjohn; US 3944595; 1976; Chem.Abstr.; EN; 85; 176939.

Ref. 5

2968330; Patent; Upjohn; US 3933895; 1974; Chem.Abstr.; EN; 85; 62726.

Ref. 6

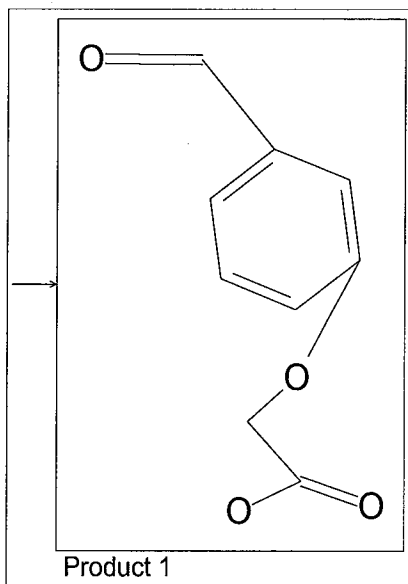
4384558; Patent; The Upjohn Co.; US 3933896; 1976; Chem.Abstr.; EN; 85; 32508.

Ref. 7

3007991; Patent; Upjohn Comp.; US 3928417; 1975; Chem.Abstr.; EN; 85; 77744.

Ref. 8

4171729; Patent; The Upjohn Co.; DE 2209990; 1972; Chem.Abstr.; EN; 78; 29477.



## Reaction 13 of 17

Reaction ID

Reactant BRN

Product BRN

No. of Reaction Details

Reaction Classification

Solvent

Other Conditions

Find similar reactions

9811771

2048742 (3-formyl-phenoxy)-acetic acid

750077 1-(triphenyl- $\lambda^5$ -phosphanylidene)-propan-2-one

9906109 [3-(3-oxo-but-1-enyl)-phenoxy]-acetic acid

1

Preparation

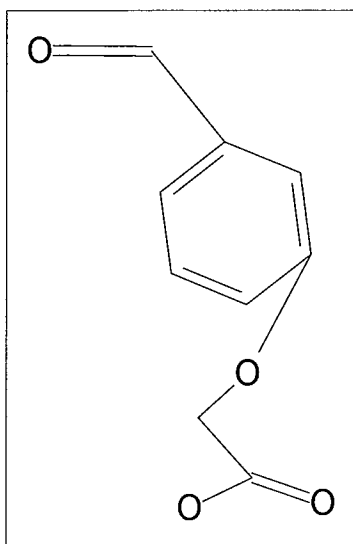
tetrahydrofuran

Heating

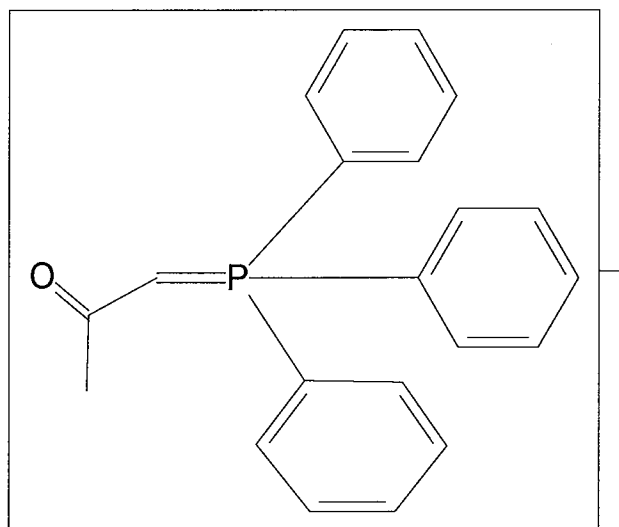
[\*\*click here\*\*](#)

Ref. 1

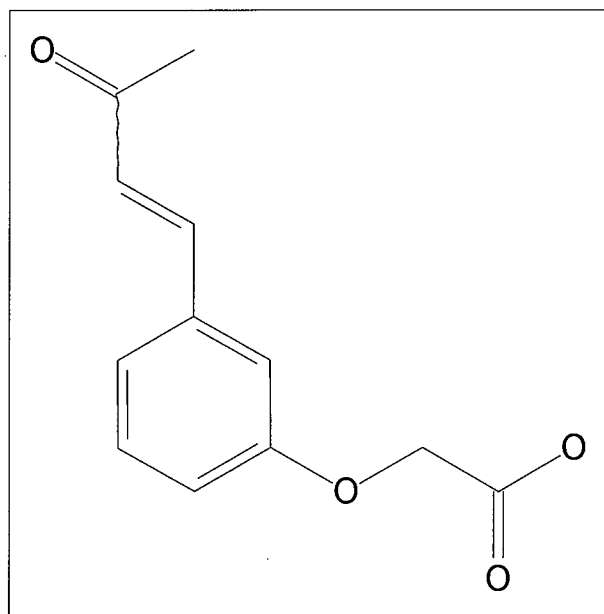
6486678; Journal; Acton, John J.; Black, Regina M.; Jones, A. Brian;



Reactant 1



Reactant 2



Product 1

## Reaction 14 of 17

Reaction ID

**9968144**

Reactant BRN

**507099** 3-hydroxy-benzaldehyde

Product BRN

**506256** bromoacetic acid methyl ester

No. of Reaction Details

1

Reaction Classification

Multistage

No. of Stages

2

Stage 1

Stage 2

Reagent

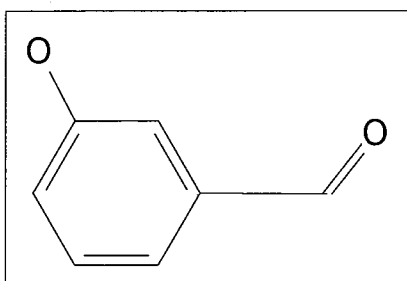
sodium hydroxide

Find similar reactions

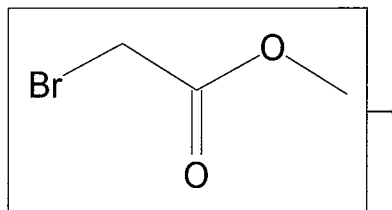
[click here](#)

Ref. 1

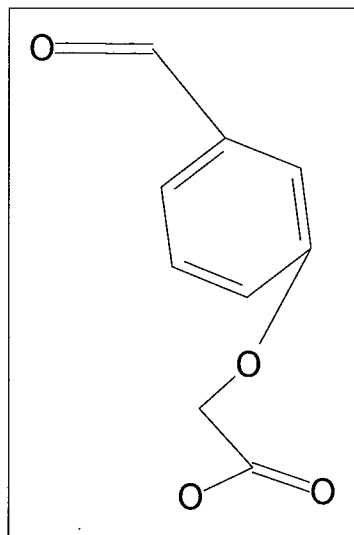
**6502017**; Journal; Belokon', Yuri N.; Carta, Paola; North, Michael; TELEAY; Tetrahedron Lett.; EN; 46; 26; 2005; 4483 - 4486.



Reactant 1



Reactant 2



Product 1

## **Reaction 15 of 17**

Reaction ID

Reactant BRN

Product BRN

No. of Reaction Details

Reaction Classification

No. of Stages

Stage 1

Stage 2

Stage Reactant BRN

Find similar reactions

**9969154**

**2048742** (3-formyl-phenoxy)-acetic acid

**1902903** Trimethylsilyldiazomethan

**507066** propionic acid anhydride

**4652394** hydrocyanic acid; potassium salt

**10079086** propionic acid cyano-(3-methoxycarbonylmethoxy-phenyl)-methyl ester

1

Multistage

2

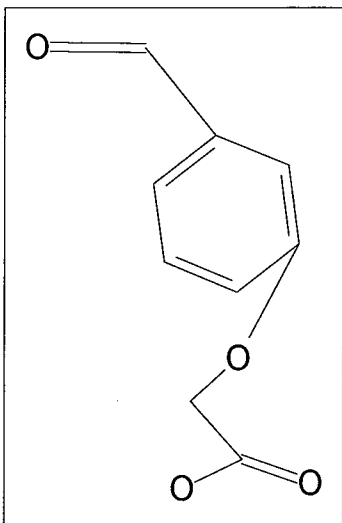
**507066** propionic acid anhydride

**4652394** hydrocyanic acid; potassium salt

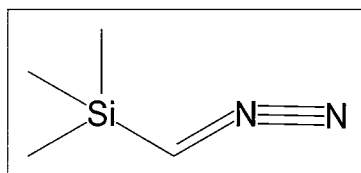
[click here](#)

Ref. 1

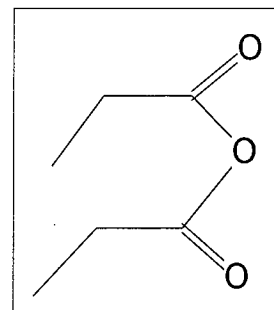
**6502017**; Journal; Belokon', Yuri N.; Carta, Paola; North, Michael; TELEAY; Tetrahedron Lett.; EN; 46; 26; 2005; 4483 - 4486.



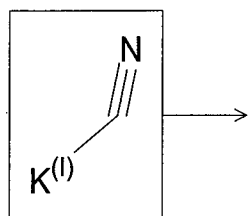
Reactant 1



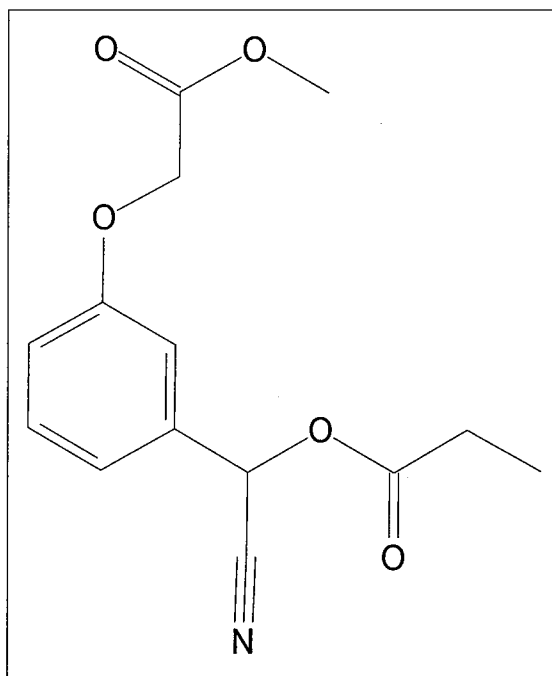
Reactant 2



Reactant 3



Reactant 4



Product 1

## Reaction 16 of 17

Reaction ID

Reactant BRN

Product BRN

No. of Reaction Details

Reaction Classification

Find similar reactions

**9969155**

**2048742** (3-formyl-phenoxy)-acetic acid

**507066** propionic acid anhydride

**1902903** Trimethylsilyldiazomethan

**4652394** hydrocyanic acid; potassium salt

**10082151** propionic acid cyano-(3-methoxycarbonylmethoxy-phenyl)-methyl ester

**10082152** propionic acid cyano-(3-methoxycarbonylmethoxy-phenyl)-methyl ester

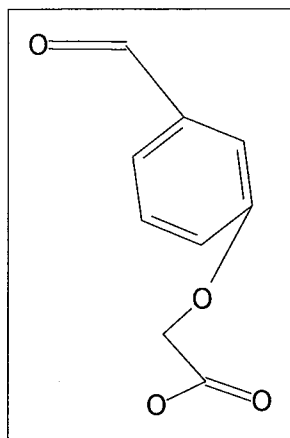
1

Preparation

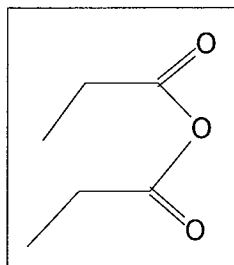
[\*\*click here\*\*](#)

Note 1  
Ref. 1

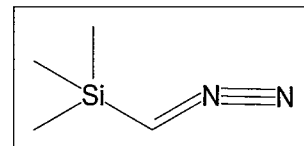
Multistep reaction. Title compound not separated from byproducts  
**6502017**; Journal; Belokon', Yuri N.; Carta, Paola; North, Michael;  
TELEAY; Tetrahedron Lett.; EN; 46; 26; 2005; 4483 - 4486.



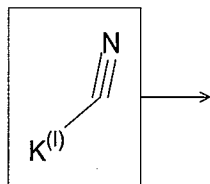
Reactant 1



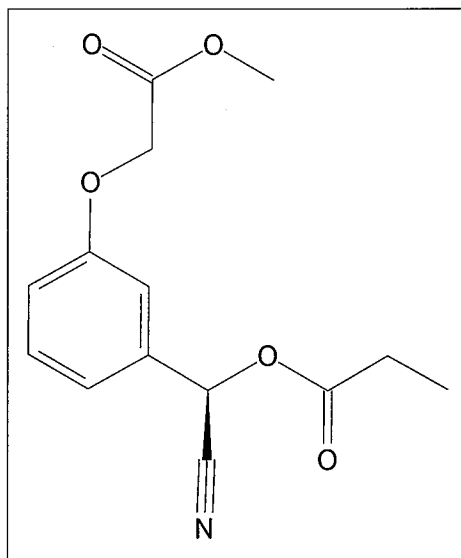
Reactant 2



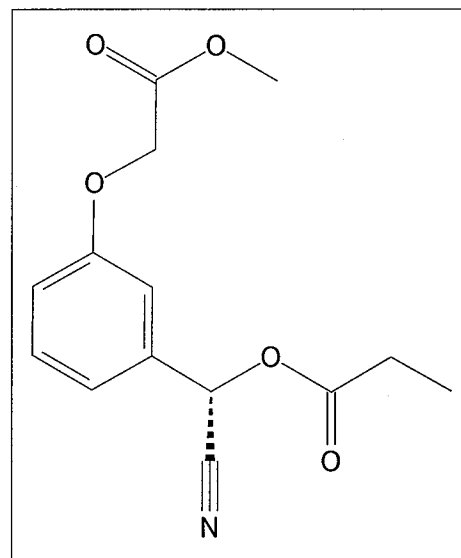
Reactant 3



Reactant 4



Product 1



Product 2

## Reaction 17 of 17

Reaction ID  
Reactant BRN

Product BRN

No. of Reaction Details  
Reaction Classification  
Yield  
Reagent  
Solvent  
Other Conditions  
Find similar reactions

**10200266**

**195229** 1,3,6-trimethyl-5-nitro-1*H*-pyrimidine-2,4-dione

**2048742** (3-formyl-phenoxy)-acetic acid

**10375693** {3-[2-(1,3-dimethyl-5-nitro-2,6-dioxo-1,2,3,6-tetrahydro-  
pyrimidin-4-yl)-vinyl]-phenoxy}-acetic acid

1

Preparation

55 percent (BRN=10375693)

piperidine

dioxane

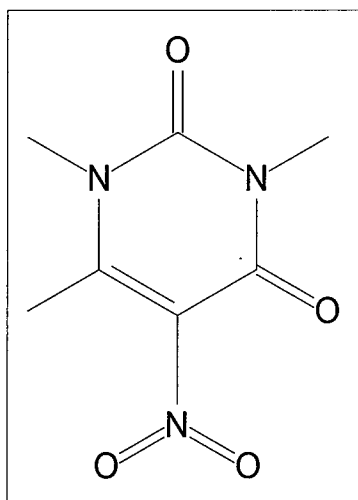
Heating

[\*\*click here\*\*](#)

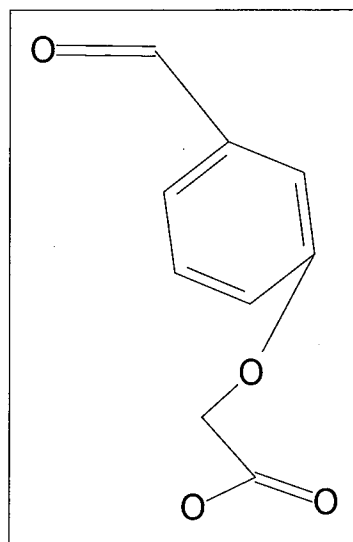
Ref. 1

**6562381**; Journal; Carotti, Angelo; Cadavid, Maria Isabel; Centeno, Nuria B.; Esteve, Cristina; Loza, Maria Isabel; Martinez, Ana; Nieto, Rosa; Ravina, Enrique; Sanz, Ferran; Segarra, Victor; Sotelo, Eddy;

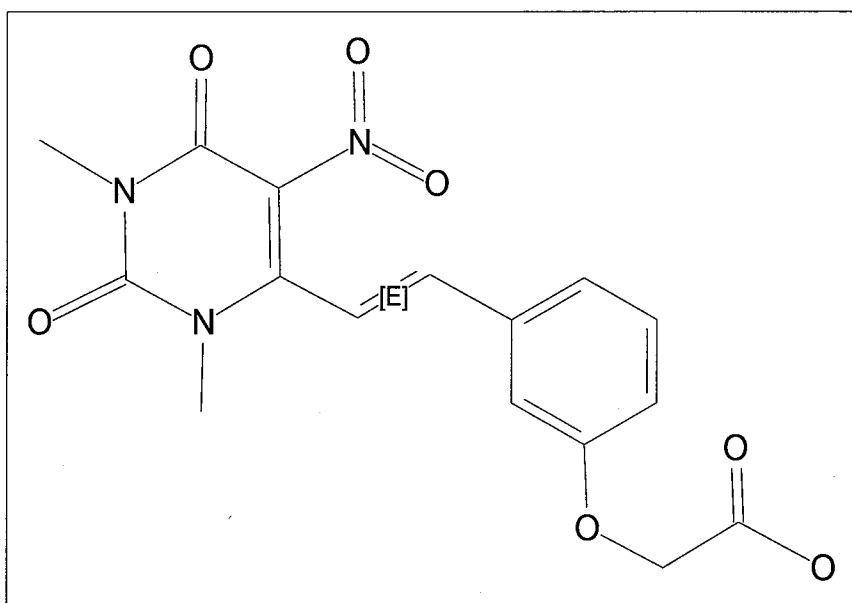




Reactant 1



Reactant 2



Product 1

## Derivative 1 of 4

Note 1  
Ref. 1

Semicarbazon: F:212-213.5grad (Zers.)  
**4162241**; Journal; Krassowska et al.; PRCHAB; Przem. Chem.; 52;  
1973; 741,742,743.

## Derivative 2 of 4

Note 1  
Ref. 1

Thiosemicarbazon: F:203-204grad  
**4162241**; Journal; Krassowska et al.; PRCHAB; Przem. Chem.; 52;  
1973; 741,742,743.

## Derivative 3 of 4

Note 1 2,4-Dinitrophenylhydrazon: F:251.5-252.5grad  
Ref. 1 **4162241**; Journal; Krassowska et al.; PRCHAB; Przem. Chem.; 52; 1973; 741,742,743.

## Derivative 4 of 4

Note 1 Ethylester: Kp(2):148-150grad  
Ref. 1 **4162241**; Journal; Krassowska et al.; PRCHAB; Przem. Chem.; 52; 1973; 741,742,743.

## Crystal Property Description

Colour & Other Properties Nadeln

Note 1 Handbook  
Ref. 1 **1970630**; Journal; Elkan; CHBEAM; Chem. Ber.; 19; 1886; 3051.

## Melting Point 1-5

VALUE (MP) C	Solvent (.SOL)	Entry Date	Note	Ref.
148 124 - 126 114 - 117 114 - 116 112.5 - 113.5	H2O		1	1 2 3-7 8 9

Note 1 Handbook  
Ref. 1 **1970630**; Journal; Elkan; CHBEAM; Chem. Ber.; 19; 1886; 3051.  
Ref. 2 **4068762**; Patent; Biorex Lab. Ltd.; DE 2810253; 1978; Chem.Abstr.; EN; 90; 22628.  
Ref. 3 **2893918**; Patent; Upjohn; US 3944595; 1976; Chem.Abstr.; EN; 85; 176939.  
Ref. 4 **2968330**; Patent; Upjohn; US 3933895; 1974; Chem.Abstr.; EN; 85; 62726.  
Ref. 5 **4384558**; Patent; The Upjohn Co.; US 3933896; 1976; Chem.Abstr.; EN; 85; 32508.  
Ref. 6 **3007991**; Patent; Upjohn Comp.; US 3928417; 1975; Chem.Abstr.; EN; 85; 77744.  
Ref. 7 **4171729**; Patent; The Upjohn Co.; DE 2209990; 1972; Chem.Abstr.; EN; 78; 29477.  
Ref. 8 **4084581**; Patent; Ciba-Geigy; DE 2209128; 1972; Chem.Abstr.; EN; 78; 5413.  
Ref. 9 **4162241**; Journal; Krassowska et al.; PRCHAB; Przem. Chem.; 52; 1973; 741,742,743.

## IR Spectroscopy

Description Bands

Ref. 1 **4162241**; Journal; Krassowska et al.; PRCHAB; Przem. Chem.; 52;

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### **Reference 5 of 16**

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### **Reference 6 of 16**

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### **Reference 7 of 16**

4068762; Patent; Biorex Lab. Ltd.; DE 2810253; 1978; Chem.Abstr.; EN; 90; 22628.

### **Reference 8 of 16**

4084581; Patent; Ciba-Geigy; DE 2209128; 1972; Chem.Abstr.; EN; 78; 5413.

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### **Reference 10 of 16**

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### **Reference 11 of 16**

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